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Discrete element simulations of hot pressing of intermetallic matrix composites

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Uniaxial hot pressing is a common technology of powder metallurgy integrating the processes of powder compaction and sintering. Hot pressing is mostly used to manufacture hard and brittle materials, such as ceramics, intermetallics and metal matrix composites, where a high density must be guaranteed. Sintering is the essential stage of a PM process consisting of the consolidation of particulate material at high temperatures but below the melting point. As a result of the sintering process, a solid compact body is formed from the powder. The material microstructure during sintering undergoes changes due to particle compaction and rearrangement, generation and growth of cohesive bonds, leading to the reduction and elimination of porosity. The processes at the microscopic scale induce changes in the macroscopic physical properties.

Great progress in the technology of sintering and powder metallurgy techniques enables the permanent development of modern materials, such as composites—materials formed from two (or more) components (e.g., metallic, intermetallic or ceramic) with different physical and chemical properties, which together give different and usually improved characteristics with respect to individual components. The manufacturing of intermetallic matrix composites is a complex and nontrivial issue. Residual stresses and material cracking in composites are typical defects due to the differences in the atomic structure and properties between intermetallics and ceramic materials, but there are also other additional difficulties in the sintering of mixed powders in comparison to those encountered in the sintering of a single phase powder. Possible chemical interactions between phases, different sinterability, different particle sizes, sintering process parameters, including heating rate, sintering temperature, and time, are factors which should be carefully considered in the design of a sintering process for mixed powders.

The manufacturing process of hot pressing can be modeled as the combination of the two subsequent main stages: the initial powder compaction and pressure-assisted sintering. Generally, the sintering of granular material is a very complex process, affected by many factors, and therefore it is difficult for modeling. Recently, sintering models have been successfully implemented within the discrete element method. Discrete models take into account the discontinuities, defects and particle size. Discrete modeling has been developed in response to the deficiency of a continuous model associated with the inability to consider all kind of defects in the material, and the difficulties in formulating constitutive equations of those models. The discrete element method (DEM), which has been applied in this research, is based on a discrete element representation of the compacted powder, which is modeled by a large collection of rigid or deformable discrete elements interacting among one another with contact forces.

This work presents numerical modeling of a hot pressing process of a two-phase powder mixture validated with our own experimental results. The original DEM model, which was applied in the simulation of the one-phase hot pressing process, is now extended to model a powder metallurgy process of an intermetallic composite specimen. Unlike other discrete element models of the two-phase powder mixture, which were only focused on the sintering process, our approach allows us to model the entire process of powder metallurgy with its subsequent steps, starting from the initial compaction of the powder by uniaxial loading, through subsequent consolidation during sintering, and finally, ending up with the cooling of the sintered material and unloading. The present study is one of the first efforts of discrete element modeling of two-phase sintering accounting for more than one type of interparticle interaction. Special emphasis has been placed on the interaction between the intermetallic and ceramic particles by formulating a special model for the adhesive contact bond.

The numerical investigation has been carried out for a powder metallurgy process performed to manufacture a composite with the NiAl intermetallic matrix reinforced with Al2O3 ceramics. The discrete element model has been generated using a special procedure which ensures a random spatial distribution of powder particles of each phase. The generation algorithm allows us to satisfy the main requirements of a real two-phase powder after mixing and compaction, such as the isotropy of composite material and the uniform distribution of reinforcement (ceramic) particles in the intermetallic NiAl matrix. This should also be highlighted in the context of the previously mentioned papers. Own experimental results were used to calibrate and validate the numerical model. The model was calibrated by fitting the numerical densification curve to the experimental data for a given set of process parameters. Finally, the calibrated model was validated by numerical simulations performed for different process parameters and by comparing the numerical and experimental results.

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